

Analysis and identification of quantum dynamics using Lie algebra homomorphisms and Cartan decompositions

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Abstract

In this paper, we consider the problem of model equivalence for quantum systems. Two models are said to be (input-output) equivalent if they give the same output for every admissible input. In the case of quantum systems, the output is the expectation value of a given observable or, more in general, a probability distribution for the result of a quantum measurement. We link the input-output equivalence of two models to the existence of a homomorphism of the underlying Lie algebra. In several cases, a Cartan decomposition of the Lie algebra $su(n)$ is useful to find such a homomorphism and to determine the classes of equivalent models. We consider in detail the important cases of two level systems with a Cartan structure and of spin networks. In the latter case, complete results are given generalizing previous results to the case of networks of spin particles with any value of the spin. In treating this problem, we prove some instrumental results on the subalgebras of $su(n)$ which are of independent interest.

Keywords: Quantum Control Systems, Parameter Identification, Lie Algebraic Methods, Spin Systems.

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1 Introduction

Dynamical models of quantum systems have been recently the subject of investigation, concerning their structural properties, by use of methods of control theory. Appropriate definitions of controllability and observability of quantum systems have been given and practical conditions to check these properties have been proposed (see e.g. [1], [6], [10], [11]). In many cases, the tools used are the ones of Lie algebra and Lie group theory. Information on the properties of the dynamics is obtained by a study of the structure of a Lie algebra associated to the system and how this relates to the particular equations at hand. This geometric approach has proved useful not only to analyze the dynamics but also to design control laws. This approach can also be used to study problems of parameter identification of quantum systems and this is the subject of the present paper. In particular, the problem we shall study is the classification of models of quantum systems whose behavior cannot be distinguished by an external observer. We shall call these models (*input-output*) *equivalent*. This problem is motivated by several experimental scenarios. In particular consider a molecule which is a network of particles with spin with all the other degrees of freedom neglected. A model Hamiltonian is associated to this system in which parameters modeling the interaction between particles as well as the interaction with an external electro-magnetic field are unknown. Also, the initial state of the system might be unknown. In experimental scenarios such as Nuclear Magnetic Resonance and Electron Paramagnetic Resonance, it is possible to drive the system with a magnetic field and measure the expectation value of a given observable, for example the total spin in a given direction. The question of fundamental and practical importance is to what extent, with this type of experiments, it is possible to distinguish between different models. As we shall see in this

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paper, this question is related to the existence of a particular Lie algebra homomorphism which relates the equations of the two models.

The main results of this paper are the solution of the model equivalence problem for a class of two level systems in Theorem 2, a number of auxiliary results (Theorems 4-6) on the structure of the Lie algebra $su(n)$ and its subalgebras and Theorem 7 where we completely solve the problem of characterizing equivalent models for networks of spin. The latter result generalizes results previously obtained in [2] and [7], which were proven only for networks of spin $\frac{1}{2}$ and 1's, to networks of interacting spins of any value and where the spin itself is an unknown parameter to be identified. A further motivation for this research can be found in [14] where it was shown that thermodynamic methods commonly used to identify the parameters of spin networks such as in molecular magnets [3], [5] are not always adequate. The generalization presented in this paper is obtained through a Cartan decomposition technique recently presented in [8] which helps determining the homomorphism between equivalent models in the form of a Cartan involution.

The paper is organized as follows. In Section 2, we describe the problem of model equivalence for quantum systems. In Section 3, we link the equivalence of two models to the existence of an appropriate Lie algebra homomorphism. In several cases the structure of the dynamics is related to a Cartan decomposition of $su(n)$ and suggests the form of such a homomorphism as well as of the classes of equivalent models. We give a two level example in Section 4 and treat the case of general spin networks in Section 5. Instrumental to the solution of the model equivalence problem for spin networks are some results of independent interest concerning the existence of subalgebras of $su(n)$ with specific features. The proofs of these results are presented in Section 6. Concluding remarks are given in Section 7.

2 The problem of model equivalence for quantum systems

Consider a model Hamiltonian for a quantum system, $H(t) := H(u(t))$, where, in a semi-classical description, the dependence on time is due to the interaction with external fields, $u := u(t)$, which play the role of *controls*. The evolution of the state of the system, described by a density matrix $\rho := \rho(t)$, is determined, other than by H , by the initial state $\rho(0) = \rho_0$. In particular, ρ is the solution of the Liouville's equation

$$\dot{\rho} = [-iH, \rho], \quad (1)$$

with initial condition $\rho(0) = \rho_0$. For this system, we measure an observable S . Considering, for simplicity, a Von Neumann-Lüders measurement³, writing S in terms of orthogonal projections

$$S := \sum_j \lambda_j \Pi_j, \quad (2)$$

the probability of having a result λ_j , when the state is ρ , is given by

$$P_j := Tr(\Pi_j \rho). \quad (3)$$

As the probabilities P_j are the only information that can be gathered by an external observer, it is motivated to ask what classes of models $\{H(u), \rho_0\}$ will give the same probabilities, for any functional form of the control u . In other terms, we ask what classes of models are

³Natural extensions can be made to general measurements [4] for the related issue of observability of quantum systems.

indistinguishable by experiments that involve driving the system with controls, in a given set of functions, and measuring a given observable. These models will be called *(Input-Output) Equivalent*.

It is appropriate to treat the case where the *expectation value* of the measurable S , i.e. the ‘output’,

$$y := \text{Tr}(S\rho), \quad (4)$$

is measured. Not only this is the case in several experimental situations, such as nuclear magnetic resonance, but it is not a significant restriction as compared to the case where the probabilities (3) are considered. As the structure of the output (4) is the same as the one of the outputs (3), the passage from the treatment for the expectation value to the one for probabilities corresponds to extending a single output treatment to a multiple output treatment. This can be accomplished without difficulties.

In order to render the problem of characterizing the classes of equivalent models treatable, we need to assume some structure on the Hamiltonian H . This corresponds to the passage from *unstructured uncertainty* to *parametric uncertainty* often discussed in identification theory (see e.g. [13]). In particular, it is often the case that the Hamiltonian $H = H(u)$ has the bilinear form

$$H := H_0 + \sum_{j=1}^m H_j u_j(t), \quad (5)$$

for some control functions u_1, \dots, u_m , and *internal Hamiltonian* H_0 and *interaction Hamiltonians* H_j ’s, $j = 1, \dots, m$. These can be considered as Hermitian matrices of dimension n , i.e. elements of $isu(n)$, where n is the dimension of the system, assumed finite. Moreover, in many cases, H_0 and the H_j ’s belong to two orthogonal complementary subspaces of $isu(n)$ corresponding to a Cartan decomposition of $su(n)$ [9]. These are two subspaces $i\mathcal{K}$ and $i\mathcal{P}$, such that the subspaces of $su(n)$, \mathcal{K} and \mathcal{P} , satisfy the commutation relations

$$[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}, \quad [\mathcal{K}, \mathcal{P}] \subseteq \mathcal{P}, \quad [\mathcal{P}, \mathcal{P}] \subseteq \mathcal{K}. \quad (6)$$

If the system is a multipartite system, every H_j is a linear combination of Hamiltonians modeling the interaction of each individual system with the external field. In matrix notation, H_j is a linear combination of elements of the type $\mathbf{1} \otimes \mathbf{1} \otimes \dots \otimes \mathbf{1} \otimes L \otimes \mathbf{1} \otimes \dots \otimes \mathbf{1}$, where L is an Hermitian matrix of appropriate dimensions and all the other places are occupied by identities $\mathbf{1}$. Also, H_0 is very often a linear combination of elements modeling the interaction between two subsystems, which can be written as tensor products of matrices equal to the identity except in two locations. In these cases the relevant Cartan decomposition for the Hamiltonian (5) can often be chosen of the *odd-even type* described in the recent paper [8]. Also if S is a sum of observables on each individual subsystem, i.e. total angular momentum (see e.g. [12]), it can always be written as sum of tensor products all equal to the identity except in one position. In these cases iS , belongs to one of the subspaces of the Cartan decomposition⁴.

In the following, we shall consider, as standing assumption, only finite dimensionality of the Hamiltonian H and the bilinear form (5) and will make precise the assumptions on the Cartan structure of the Hamiltonian when needed.

⁴Notice that the situation may be different if we consider the case of a single output given by the expectation value (4) and the case of several outputs given by the probabilities in (3).

3 Model equivalence and Lie algebra homomorphisms

Consider two models with Hamiltonian of the form (5) and output of the form (4)

$$\dot{\rho} = [-i(H_0 + \sum_{j=1}^m H_j u_j), \rho], \quad \rho(0) = \rho_0, \quad y = \text{Tr}(S\rho), \quad (7)$$

$$\dot{\rho}' = [-i(H'_0 + \sum_{j=1}^m H'_j u_j), \rho'], \quad \rho'(0) = \rho'_0, \quad y' = \text{Tr}(S'\rho'). \quad (8)$$

The following theorem links the existence of an appropriate Lie algebra homomorphism to the equivalence of the two models.

Theorem 1 *Let n and n' be the dimensions of the two models (7), (8), respectively. Let ϕ be a homomorphism, $\phi : u(n) \rightarrow u(n')$, and ϕ^* its dual with respect to the standard inner product $\langle A, B \rangle := \text{tr}(AB^*)$. Assume*

$$-iH'_0 = \phi(-iH_0), \quad -iH'_j = \phi(-iH_j), \quad \phi^*(iS') = iS. \quad (9)$$

Then if $i\rho'_0 = \phi(i\rho_0)$ the models are equivalent. Viceversa, if the models are equivalent and (8) is observable, then

$$i\rho'_0 = \phi(i\rho_0). \quad (10)$$

Proof. Multiply (7) and (8) by i and then apply ϕ to the equation obtained from (7). Combining the two resulting equations, we obtain

$$\frac{d}{dt}(i\rho' - \phi(i\rho)) = [\phi(-iH_0) + \sum_j \phi(-iH_j)u_j, i\rho' - \phi(i\rho)]. \quad (11)$$

Now, if (10) is verified, then $i\rho'(t) = \phi(i\rho(t))$, for every t and for every control. Therefore we have

$$\text{Tr}(S'\rho') = \text{Tr}(-iS'i(\rho')) = \text{Tr}(-iS'\phi(i\rho)) = \text{Tr}(\phi^*(-iS')i\rho) = \text{Tr}(S\rho), \quad (12)$$

and the two models are equivalent. Viceversa, assume the two models are equivalent. From (12), we have

$$\text{Tr}(iS'(i\rho' - \phi(i\rho))(t)) = 0, \quad (13)$$

for every t . Writing the solution of (11) as $(i\rho' - \phi(i\rho))(t) = X(i\rho' - \phi(i\rho))(0)X^*$, where X is the solution of the (Schrödinger) operator equation $\dot{X} = (\phi(-iH_0) + \sum_j \phi(-iH_j)u_j)X$, $X(0) = \mathbf{1}$, we have

$$\text{Tr}(X^*iS'X(i\rho'_0 - \phi(i\rho_0))) = 0. \quad (14)$$

As the system (8) is observable, we have that $X^*iS'X$ span all of $su(n')$, which implies $i\rho'_0 = \phi(i\rho_0)$. \square

As we shall show in the remainder of the paper (cf. also [2]), it is possible for cases of physical interest to give a stronger version of Theorem 1. In particular, it is possible to show that the existence of a homomorphism ϕ satisfying (9) is also necessary for equivalence of two models. This way, we can characterize all the classes of equivalent models in terms of homomorphisms. We shall do this for a two level example in the next section and general spin networks in Section 5. In both cases we exploit a Cartan decomposition underlying the dynamics of the models. In general, more structure will have to be assumed to avoid trivial cases. For example, if $S = S'$ is a scalar matrix, then every two models are equivalent. To avoid this case, a reasonable extra assumption is the observability of the two models. Also,

we need to assume that the initial states are not both perfect mixtures, otherwise, with $S = S'$, the output for any two equivalent models will be the same, independently of the dynamics. Moreover $-iH_j$ and $-iH'_j$, $j = 0, \dots, m$, may be in general assumed traceless, as the trace only adds an extra common phase factor to the dynamics, which cannot be detected.

4 Model equivalence of two level systems

Consider a spin $\frac{1}{2}$ particle which is driven by an electro-magnetic control field along the z axis, interacts with a constant unknown magnetic field along a (unknown) direction in the $x - y$ plane and has unknown initial state. The practical question is to what extent, by driving the system with the control field and measuring the average value of the spin magnetization in the z direction, it is possible to obtain information about the unknown parameters of the system. This type of model has a Cartan structure which is shared by several other models of physical interest and is instrumental in finding a homomorphism between equivalent models. We describe this below.

The Lie algebra $su(2)$, which is the relevant Lie algebra in the two level case, has, up to conjugacy, only one Cartan decomposition (or in other terms all the types of decompositions coincide in this case) which corresponds to the classical Euler decomposition of the Lie group $SU(2)$ [9]. This extends to a decomposition of $u(2)$ which can always be written, as

$$u(2) = \mathcal{K} \oplus \mathcal{P}. \quad (15)$$

Here \mathcal{K} and \mathcal{P} satisfy the commutation relations in (6) and are given, up to conjugacy, by

$$\mathcal{K} := \text{span}\{i\sigma_z\}, \quad \mathcal{P} := \text{span}\{i\sigma_x, i\sigma_y, i\mathbf{1}_{2 \times 2}\}, \quad (16)$$

where $\mathbf{1}_{2 \times 2}$ is the 2×2 identity matrix and σ_x , σ_y and σ_z are the Pauli matrices

$$\sigma_x := \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \frac{1}{2} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_z := \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (17)$$

The dynamical and output equation, for the above model of a spin $\frac{1}{2}$ particle in an electro-magnetic field, can be written as

$$\dot{\rho} = [A + i\sigma_z u(t), \rho], \quad y = \text{Tr}(\sigma_z \rho), \quad \rho(0) = \rho_0, \quad (18)$$

where ρ_0 is an unknown initial density matrix and $A := xi\sigma_x + yi\sigma_y$, with x and y unknown. This model has a *Cartan structure* in that A is in \mathcal{P} and $i\sigma_z$ (the control and observation part) is in \mathcal{K} , with \mathcal{K} and \mathcal{P} defined in (16). We assume $x^2 + y^2 \neq 0$ which implies controllability and therefore observability [6] for this model. The following result characterizes all the classes of equivalent models in terms of Lie algebra homomorphisms.

Theorem 2 *Consider two models*

$$\dot{\rho} = [A + i\sigma_z u(t), \rho], \quad y = \text{Tr}(\sigma_z \rho), \quad \rho(0) = \rho_0, \quad (19)$$

$$\dot{\rho}' = [A' + i\sigma_z u(t), \rho], \quad y = \text{Tr}(\sigma_z \rho'), \quad \rho'(0) = \rho'_0, \quad (20)$$

with ρ_0 and ρ'_0 not both equal to scalar matrices (representing perfect mixtures) and A and A' given by

$$A := xi\sigma_x + yi\sigma_y, \quad \text{and} \quad A' := x'i\sigma_x + y'i\sigma_y. \quad (21)$$

Assume

$$x^2 + y^2 \neq 0 \text{ and } x'^2 + y'^2 \neq 0. \quad (22)$$

Then the two models are equivalent if and only if there exists an automorphism $\phi : u(2) \rightarrow u(2)$ with

$$\phi^*(i\sigma_z) = i\sigma_z \quad (23)$$

and

$$A' = \phi(A), \quad \phi(i\sigma_z) = i\sigma_z, \quad i\rho'_0 = \phi(i\rho_0). \quad (24)$$

Proof. It is clear that if the automorphism ϕ exists, satisfying (23) (24), the two models are equivalent. This follows from a direct application of Theorem 1. To prove the opposite, first notice that, from the equivalence assumption, we have

$$y(t) := \text{Tr}(\sigma_z \rho(t)) = \text{Tr}(\sigma_z \rho'(t)) := y'(t), \quad (25)$$

for every $t \geq 0$ and every admissible control.

We consider an inner automorphism ϕ of the following type

$$\phi(L) := e^{-i\alpha\sigma_z} L e^{i\alpha\sigma_z}, \quad L \in u(n), \quad (26)$$

as α varies in \mathbf{R} .

Clearly (23) and the second one of (24) are verified for any $\alpha \in \mathbf{R}$. Moreover

$$\phi(A) = \bar{x}i\sigma_x + \bar{y}i\sigma_y, \quad (27)$$

with

$$\begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix} = K_\alpha \begin{pmatrix} x \\ y \end{pmatrix}, \quad (28)$$

and

$$K_\alpha := \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix}. \quad (29)$$

Also, if we write

$$i\rho_0 := \rho_x i\sigma_x + \rho_y i\sigma_y + \rho_z i\sigma_z + \frac{1}{2}i\mathbf{1}, \quad (30)$$

$$i\rho'_0 := \rho'_x i\sigma_x + \rho'_y i\sigma_y + \rho'_z i\sigma_z + \frac{1}{2}i\mathbf{1}$$

we have

$$\phi(i\rho_0) = \bar{\rho}_x i\sigma_x + \bar{\rho}_y i\sigma_y + \bar{\rho}_z i\sigma_z + \frac{1}{2}i\mathbf{1}, \quad (31)$$

with

$$\begin{pmatrix} \bar{\rho}_x \\ \bar{\rho}_y \end{pmatrix} = K_\alpha \begin{pmatrix} \rho_x \\ \rho_y \end{pmatrix}. \quad (32)$$

Using the equivalence assumption (25) at $t = 0$ we immediately obtain

$$\rho_z = \rho'_z. \quad (33)$$

Moreover, differentiating (25) using the dynamical equations (19) (20), we obtain

$$\text{Tr}(\rho[\sigma_z, A]) = \text{Tr}(\rho'[\sigma_z, A']). \quad (34)$$

Writing this at time $t = 0$ and using the definitions (21) and (30) along with the commutation relation for the Pauli matrices

$$[i\sigma_x, i\sigma_y] = i\sigma_z, \quad [i\sigma_y, i\sigma_z] = i\sigma_x, \quad [i\sigma_z, i\sigma_x] = i\sigma_y, \quad (35)$$

we obtain

$$\rho_y x - \rho_x y = \rho'_y x' - \rho'_x y'. \quad (36)$$

Differentiating (34) and using the fact that the resulting equation has to be valid for every value of the control, we obtain the two equations

$$Tr(\sigma_z[A, [A, \rho]]) = Tr(\sigma_z[A', [A', \rho']]), \quad (37)$$

and

$$Tr(i\sigma_z[A, [\sigma_z, \rho]]) = Tr(i\sigma_z[A', [\sigma_z, \rho']]). \quad (38)$$

From equation (38), as for equation (36), we obtain

$$x\rho_x + y\rho_y = x'\rho'_x + y'\rho'_y. \quad (39)$$

From equation (37), we obtain

$$(x^2 + y^2)Tr(\sigma_z\rho) = (x'^2 + y'^2)Tr(\sigma_z\rho'). \quad (40)$$

Using the fact that $Tr(\sigma_z\rho)$ is not always zero (because of the controllability condition (22))⁵ and equation (25), we have

$$x^2 + y^2 = x'^2 + y'^2. \quad (42)$$

Therefore, for some α , we can write

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = K_\alpha \begin{pmatrix} x \\ y \end{pmatrix}, \quad (43)$$

with K_α in (29), and this, compared with (28) and (27), gives the first one of (24). To obtain the third one (with the same ϕ), we recall (22) that $x^2 + y^2 \neq 0$. Letting $J := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ and using (43), we can write (36) and (39), respectively, as

$$[x, y]J[\rho_x, \rho_y]^T = [x, y]K_\alpha^T J[\rho'_x, \rho'_y]^T, \quad (44)$$

$$[x, y][\rho_x, \rho_y]^T = [x, y]K_\alpha^T [\rho'_x, \rho'_y]^T. \quad (45)$$

Since K_α^T commutes with J , we can write these as

$$\begin{pmatrix} [x, y]J \\ [x, y] \end{pmatrix} [\rho_x, \rho_y]^T = \begin{pmatrix} [x, y]J \\ [x, y] \end{pmatrix} K_\alpha^T [\rho'_x, \rho'_y]^T. \quad (46)$$

Since $x^2 + y^2 = -\det \begin{pmatrix} [x, y]J \\ [x, y] \end{pmatrix} \neq 0$, we can write

$$[\rho'_x, \rho'_y]^T = K_\alpha [\rho_x, \rho_y]^T, \quad (47)$$

⁵From controllability (22), we cannot have

$$Tr(\sigma_z\rho(t)) \equiv Tr(\sigma_z\rho'(t)) \equiv 0, \quad (41)$$

for every control. This would mean that, for every reachable evolution operator X , solution of the (Schrödinger) operator equation $\dot{X} = (A + i\sigma_z u)X$, $X^*\sigma_z X$ would be orthogonal to ρ_0 . However, because of controllability X may attain all the values in $SU(2)$ and therefore $X^*\sigma_z X$ span, as X varies, all of $isu(2)$. Therefore, $X^*\sigma_z X$ is always orthogonal to ρ_0 only if ρ_0 is a multiple of the identity, which we have excluded.

and therefore

$$[\rho'_x, \rho'_y] = [\bar{\rho}_x, \bar{\rho}_y], \quad (48)$$

which along with $\rho'_z = \rho_z$ gives

$$i\rho' = \phi(i\rho). \quad (49)$$

This concludes the proof of the Theorem. \square

5 Model equivalence of spin networks

5.1 Set of models of spin networks

We consider a network of n particles with spin that interact according to Heisenberg interaction. In particular, we denote the spin of the j^{th} particle by l_j and by $N_j := 2l_j + 1$ the dimension of the Hilbert space for the state of the j^{th} particle. The dimension of the Hilbert state space associated to the entire network is $N := \prod_{j=1}^n N_j$. The class of Hamiltonians we consider are of the form

$$H(t) := i(A + B_x u_x(t) + B_y u_y(t) + B_z u_z(t)), \quad (50)$$

where A , modeling the Heisenberg interaction among the particles, and $B_{x,y,z}$, modeling the interaction with external fields, are given by

$$\begin{aligned} A &:= -i \sum_{k < l, k, l=1}^n J_{kl} (I_{kx, lx} + I_{ky, ly} + I_{kz, lz}). \\ B_v &:= -i (\sum_{k=1}^n \gamma_k I_{kv}), \quad \text{for } v = x, y, \text{ or } z, \end{aligned} \quad (51)$$

respectively. Here and in the following we denote by $I_{k_1 v_1, \dots, k_r v_r}$, for $1 \leq k_1 < \dots < k_r \leq n$ and $v_j \in \{x, y, z\}$, the $N \times N$ matrix which is the Kronecker product of n matrices where in the j^{th} position we have the $N_j \times N_j$ identity if $j \notin \{k_1, \dots, k_r\}$, while if $j = k_s$ we have the $N_j \times N_j$ representation of the v_s component of spin angular momentum for a particle with spin l_j . Such matrices are given by the Pauli matrices (17) in the case where $l_j = \frac{1}{2}$ and can be calculated for every value of the spin (see e.g. [12] Section 3.5). With some abuse of notation, we shall continue denoting these matrices by σ_x , σ_y and σ_z , without explicit reference to the value of the spin. These matrices have several properties we shall use in the following. In particular, they satisfy the commutation relations (35) and

$$\sigma_x^2 + \sigma_y^2 + \sigma_z^2 = l_j(l_j + 1) \mathbf{1}_{N_j \times N_j} \quad (52)$$

(see e.g. formula (3.5.34a) in [12]).

The real scalar parameter J_{kl} in (51) is the exchange constant between particle k and particle l and the real scalar parameter γ_k is the gyromagnetic ratio of particle k . We assume that the spins of the network have all non-zero and different gyromagnetic ratios. We can associate a graph to the model, where each node represents a particle and an edge connects two nodes if and only if the corresponding exchange constant is different from zero. It is not difficult to see that if the model is controllable then, necessarily, this graph is connected. Moreover, controllability implies observability for every output of the form (4) where S is a non scalar matrix [6]. In our case, we assume to measure the expectation values of the total magnetization in the x , y , and z direction, given as in (4) where S is one of the matrices:

$$S_v := \sum_{k=1}^n I_{kv}, \quad \text{with } v \in \{x, y, z\}. \quad (53)$$

A model of the type above described will be denoted by $\Sigma := \Sigma(n, l_j, J_{kl}, \gamma_k, \rho_0)$, where the parameters $n, l_j, J_{kl}, \gamma_k, \rho_0$, which determine the model, are unknown. We will assume to have two controllable models Σ and $\Sigma' := \Sigma'(n', l'_j, J'_{kl}, \gamma'_k, \rho'_0)$ which satisfy the previous requirements and we look for necessary and sufficient conditions for these two models to be equivalent. We shall mark with a prime, ', all the quantities concerning the system Σ' .

5.2 Relevant homomorphism of $su(n)$

In [8] a method was described to construct a Cartan decomposition of the Lie algebra $su(N)$ for a multipartite system, starting from decompositions of the Lie algebras $su(N_j)$ associated to the single subsystems, each of dimension N_j , with $N := \prod_{j=1}^n N_j$. In particular, we have the following result.

Theorem 3 ([8], Section 5) *Consider a multi partite system with n subsystems of dimensions N_1, \dots, N_n . Consider the Lie algebra $u(N_j)$ related to the j -th subsystem and a Cartan decomposition*

$$u(N_j) = \mathcal{K}_j \oplus \mathcal{P}_j, \quad (54)$$

*of the type **AI** or **AII**⁶. Denote by σ_j (S_j) a generic element of an orthogonal basis of $i\mathcal{K}_j$ ($i\mathcal{P}_j$). Let the (total) Lie algebra $u(N_1 N_2 \cdots N_n)$ be decomposed as*

$$iu(N_1 N_2 \cdots N_n) = \mathcal{I}_o \oplus \mathcal{I}_e. \quad (55)$$

\mathcal{I}_o (\mathcal{I}_e) is the vector space spanned by matrices which are the tensor products of an odd (even) number of elements of the type σ_j . Then $u(N_1 N_2 \cdots N_n) = i\mathcal{I}_o \oplus i\mathcal{I}_e$ is a Cartan decomposition i.e.

$$[i\mathcal{I}_o, i\mathcal{I}_o] \subseteq i\mathcal{I}_o, \quad [i\mathcal{I}_o, i\mathcal{I}_e] \subseteq i\mathcal{I}_e, \quad [i\mathcal{I}_e, i\mathcal{I}_e] \subseteq i\mathcal{I}_o. \quad (56)$$

The decomposition (55) is called a decomposition of the *odd-even type*.

Associated to a Cartan decomposition (56) is a Cartan involution ϕ which is the identity on $i\mathcal{I}_o$ and multiplication by -1 on $i\mathcal{I}_e$. A Cartan involution is clearly a homomorphism. The structure of system (50) and (51) suggests that it is possible to choose this Cartan involution as a homomorphism mapping the equations of two equivalent models as in (9). In fact, assume that there is the same number of subsystems (spin particles) in the two models and that corresponding subsystems have the same dimension (namely the same spin). If we can display a decomposition (54) of the type **AI** or **AII** for every (spin) $su(N_j)$, such that $i\sigma_{x,y,z} \in \mathcal{K}_j$, then, for every value of the parameters, it holds that $B_{x,y,z}(') \in i\mathcal{I}_o$ and $A(') \in i\mathcal{I}_e$. As shown in the following Theorems 4-6 decompositions of this type exist. We shall see in the following subsection that the Cartan involution associated to an odd-even type Cartan decomposition is the correct homomorphism to describe classes of equivalent spin networks. In fact, not only models which are related by such a homomorphism are equivalent (according to Theorem 1) but the opposite is true as well. In other terms, two equivalent models are either exactly the same or are related through such a homomorphism.

The following three Theorems show the existence of a decomposition of $su(N_j)$ of the type **AI** or **AII** where the subalgebra \mathcal{K}_j contains the matrices $i\sigma_x, i\sigma_y$ and $i\sigma_z$. Equivalently, they show the existence of a subalgebra of $sp(\frac{N_j}{2})$ (type **AII**) or $so(N_j)$ (type **AI**) conjugate to the Lie algebra spanned by $i\sigma_x, i\sigma_y$ and $i\sigma_z$. The proofs are presented in the following section. We shall see that the situation is different for integer and half integer spins.

⁶In a decomposition **AI** $\mathcal{K}_j = so(N_j)$ and $\mathcal{P}_j = (so(N_j))^\perp$ up to conjugacy. In a decomposition **AII** $\mathcal{K}_j = sp(N_j/2)$ and $\mathcal{P}_j = (sp(N_j/2))^\perp$ up to conjugacy. [9]

Theorem 4 *If the dimension N_j of the system is even (half integer spin (Fermions)) there exists a subalgebra of $sp(\frac{N_j}{2})$ conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$ and $i\sigma_z$.*

Theorem 5 *If the dimension N_j of the system is odd (integer spin (Bosons)) there exists a subalgebra of $so(N_j)$ conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$ and $i\sigma_z$.*

Theorem 6 *If the dimension N_j of the system is even (half integer spin (Fermions)) there is no subalgebra of $so(N_j)$ conjugate to the Lie algebra spanned by $i\sigma_x$, $i\sigma_y$ and $i\sigma_z$.*

5.3 Necessary and sufficient conditions for model equivalence

In this subsection we will prove the equivalence result concerning models of spin networks. This is given by the following Theorem.

Theorem 7 *Let $\Sigma := \Sigma(n, l_j, J_{kl}, \gamma_k, \rho_0)$ and $\Sigma' := \Sigma(n', l'_j, J'_{kl}, \gamma'_k, \rho'_0)$ be two fixed models (see equations (50), (51)). Assume that both models are controllable, that for model Σ (Σ'), all the γ_k (γ'_k) are non-zero and different from each other, and that ρ_0 and ρ'_0 are not both scalar matrices. Then Σ is equivalent to Σ' i.e.:*

$$y_v(t) := Tr(S_v \rho(t)) \equiv y'_v(t) := Tr(S'_v \rho'(t)), \quad \text{for } v \in \{x, y, z\}, \quad (57)$$

and for every control u_x, u_y, u_z , if and only if the following condition holds:

Cond. (*):

1. $n = n'$
Up to a permutation of the of the set $\{1, \dots, n\}$ (i.e. a permutation of the indices for the particles)
2. $\gamma_k = \gamma'_k$,
and
- 3.

$$l_k = l'_k. \quad (58)$$

4. One of the following two conditions holds

(a)

$$A = A', \text{ and } \rho_0 = \rho'_0 \quad (59)$$

- (b) Given the Cartan involution ϕ associated to the decomposition of the odd-even type as from Theorem 3

$$A' = \phi(A), \text{ and } i\rho'_0 = \phi(i\rho_0) \quad (60)$$

The Theorem says that, under appropriate controllability assumptions, two equivalent models for spin networks are equivalent if and only they have the same number of particles, corresponding particles have the same spin, and their dynamical model and initial state are either the exactly the same or are related through the Cartan involution associated to a decomposition of the odd-even type. In practical terms, given a general spin network, by driving the network with an external electro-magnetic field and measuring the total spin in the x , y and z direction, it is, in principle, possible to identify the number of particles, their spin, the gyromagnetic ratios of every spin and the exchange constants only up to a common sign factor, if the initial state is not known. The proof that Condition (*) implies equivalence

is an application of the general property of Theorem 1. The proof that equivalence implies Condition (*) is considerably longer. However, several results can be obtained with proofs that are formal modifications of the ones presented in [2] for the special case of spin $\frac{1}{2}$ particles. We shall focus on the new part of the proof needed to generalize to the case of unknown spins.

Condition () implies equivalence*

It is clear that if (59) holds, then the two models differ possibly only by a permutation of the indices of the particles. So they are equivalent. Assume now that Condition (*) holds with (60) and assume for simplicity (and without loss of generality) that the permutation of indices is the identity. Let ϕ be the Cartan involution associated to the decomposition of the odd-even type. We notice that

$$\phi^*(iS_v) = iS_v = iS'_v, \quad v = x, y, z. \quad (61)$$

In fact, given any $C \in u(N)$, we can write $C = C_o + C_e$, with $C_o \in i\mathcal{I}_o$ and $C_e \in i\mathcal{I}_e$, it holds:

$$Tr(\phi^*(iS_v)C) := Tr((iS_v)\phi(C)) = Tr((iS_v)(C_o - C_e)) = Tr((iS_v)C_o) = Tr((iS_v)C),$$

which, since it has to hold for every C , gives (61). Equations (60) and (61) imply that equation (9) of Theorem 1 holds. Since we also have (10), from (60), we conclude that the two models are equivalent using Theorem 1.

Equivalence implies Condition ()*

The technique used in [2] to prove this result for network of spin $1/2$ particles extends to the general case treated here. However further analysis is required in this case, in particular to prove that equivalent spin networks have the same values of the spins, while in [2] it was assumed that the networks were composed by all spin $\frac{1}{2}$'s. The main reason why the proof in [2] can be extended to this case is that the basic commutation relations, which were the essential ingredient of the proofs in [2] still hold. More precisely, the matrices σ_x , σ_y and σ_z still satisfy, for every value of the spin, the commutation relations (35). This fact implies that it also holds:

$$\left[I_{k_1 v_1, \dots, k_r v_r}, I_{\bar{k} v_{\bar{k}}} \right] = \begin{cases} 0 & \text{if } \bar{k} \notin \{k_1, \dots, k_r\} \\ 0 & \text{if } \exists j \text{ with } \bar{k} = k_j \text{ and } v_{\bar{k}} = v_j \\ i I_{k_1 v_1, \dots, k_j [v_j v_{\bar{k}}], \dots, k_r v_r} & \text{if } \exists j \text{ with } \bar{k} = k_j \text{ and } v_{\bar{k}} \neq v_j \end{cases}, \quad (62)$$

independently of the values of the spins.

Assume now that the two models Σ and Σ' are equivalent. Then, using exactly the same arguments as in the proof of Proposition 4.1 of [2], we obtain that the number of the spin particle must be the same, namely $n = n'$, and, up to a permutation of the indices, $\gamma_k = \gamma'_k$, $\forall k \in \{1, \dots, n\}$, which is part 1. and 2. of Condition (*). Moreover as in Proposition 4.1 of [2], we obtain

$$Tr(I_{kv}\rho(t)) = Tr(I'_{kv}\rho'(t)), \forall k \in \{1, \dots, n\}, \forall v \in \{x, y, z\}. \quad (63)$$

Here I'_{kv} is defined as I_{kv} but for Σ' and, at this point, it may be different from I_{kv} since we have not shown yet that corresponding spins must be equal. To prove this fact, we shall use Lemma 5.1 below. The proof of this Lemma is a generalization of the proof of Lemma 5.2 in [2] where we use the general property (52) instead of the corresponding property for spin $\frac{1}{2}$'s. We postpone this proof to Appendix A.

Lemma 5.1 Assume that for all $t \geq 0$, all possible trajectories $\rho(t)$ of Σ and corresponding $\rho'(t)$ of Σ' , for fixed values $1 \leq k_1, \dots, k_r \leq n$, $v_j \in \{x, y, z\}$ and for given constants β and β' , we have:

$$\beta \text{Tr} (I_{k_1 v_1, \dots, k_r v_r} \rho(t)) = \beta' \text{Tr} (I'_{k_1 v_1, \dots, k_r v_r} \rho'(t)). \quad (64)$$

Then

1. For any pair of indices $\bar{k}, \bar{d} \in \{1, \dots, n\}$ with $\bar{k} \in \{k_1, \dots, k_r\}$ and $\bar{d} \notin \{k_1, \dots, k_r\}$,

$$\beta J_{\bar{k}\bar{d}} \text{Tr} (I_{k_1 v_1, \dots, k_r v_r, \bar{d}\bar{v}} \rho(t)) = \beta' J'_{\bar{k}\bar{d}} \text{Tr} (I'_{k_1 v_1, \dots, k_r v_r, \bar{d}\bar{v}} \rho'(t)), \quad (65)$$

for any value $\bar{v} \in \{x, y, z\}$.

2. For any pair of indices \bar{k}, \bar{d} both in $\{k_1, \dots, k_r\}$, (for example $\bar{k} = k_1, \bar{d} = k_2$) then

$$\beta (l_{\bar{d}}(l_{\bar{d}} + 1)) J_{\bar{k}\bar{d}} \text{Tr} (I_{k_1 v_1, k_3 v_3, \dots, k_r v_r} \rho(t)) = \beta' (l'_{\bar{d}}(l'_{\bar{d}} + 1)) J'_{\bar{k}\bar{d}} \text{Tr} (I'_{k_1 v_1, k_3 v_3, \dots, k_r v_r} \rho'(t)). \quad (66)$$

In words, formula (66) means that from (64), it is possible to derive a new formula as follows. Select two indices in the set $\{k_1, \dots, k_r\}$, \bar{k} and \bar{d} . One of the two indices (say \bar{d}) disappears from the subscript in the matrices I and corresponding I' . However a coefficient $l_{\bar{d}}(l_{\bar{d}} + 1)$ and $l'_{\bar{d}}(l'_{\bar{d}} + 1)$ appears in the left and right hand side, respectively, as well as a coefficient $J_{\bar{k}\bar{d}}$ and $J'_{\bar{k}\bar{d}}$.

We shall now prove that, under the assumption of equivalence, the squares of the exchange constants J_{dk} and J'_{dk} must be proportional, with a proportionality factor common to all pairs of indices d and k and this will also be instrumental in the proof of 3. of Condition (*).

Fix any $1 \leq k_1 < k_2 \leq n$, then, by applying statement 1. of Lemma 5.1, i.e. equation (65) with $\bar{k} = k_1, \bar{d} = k_2$ to equation (63) with $k = k_1$, we have:

$$J_{k_1 k_2} \text{Tr} (I_{k_1 v_1, k_2 v_2} \rho(t)) = J'_{k_1 k_2} \text{Tr} (I'_{k_1 v_1, k_2 v_2} \rho'(t)), \quad \forall v_1, v_2 \in \{x, y, z\}. \quad (67)$$

Now, to the previous equality, we apply statement 2. of Lemma 5.1, i.e. equation (66) with $\bar{k} = k_1$ and $\bar{d} = k_2$ to get:

$$(l_{k_2}(l_{k_2} + 1)) J_{k_1 k_2}^2 \text{Tr} (I_{k_1 v_1} \rho(t)) = (l'_{k_2}(l'_{k_2} + 1)) J_{k_1 k_2}'^2 \text{Tr} (I'_{k_1 v_1} \rho'(t)),$$

which, by equation (63), implies:

$$(l_{k_2}(l_{k_2} + 1)) J_{k_1 k_2}^2 = (l'_{k_2}(l'_{k_2} + 1)) J_{k_1 k_2}'^2. \quad (68)$$

Using the facts that the two indices k_1 and k_2 above are arbitrary and that the graph associated to the network is connected, by the controllability assumption, it is easy to see that there exists a positive constant $\alpha \in \mathbf{R}$ such that, for all $1 \leq d < k \leq n$:

$$J_{dk}^2 = \alpha^2 J_{dk}'^2 \quad \text{and} \quad l_k(l_k + 1) = \frac{1}{\alpha^2} l'_k(l'_k + 1). \quad (69)$$

Using (69), we can now prove 3. of Condition (*). We will do this using some lemmas and arguing by contradiction. First notice that from (69), we have that if there exists a $\bar{k} \in \{1, \dots, n\}$ such that $l_{\bar{k}} = l'_{\bar{k}}$, then necessarily $\alpha^2 = 1$, thus $l_j = l'_j$ for all $j = 1, \dots, n$, namely all the particles have the same spin. So if we assume that (58) does not hold, without loss of generality, we can assume $l_1 > l'_1$. Using equation (69), we get that $l_j > l'_j$ for all $j = 1, \dots, n$, thus also $N_j > N'_j$. Let $R := \frac{N}{N_1} = \prod_{j=2}^n N_j$ and $R' := \frac{N'}{N'_1} = \prod_{j=2}^n N'_j$.

Lemma 5.2 For all $t \in \mathbf{R}$, and all the admissible trajectories ρ and corresponding trajectory ρ' , we have:

$$\frac{\text{Tr} \left((e^{i\sigma_z t} \otimes \mathbf{1}_{R \times R}) I_{1v} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R \times R}) \rho(s) \right)}{\text{Tr} \left((e^{i\sigma_z t} \otimes \mathbf{1}_{R' \times R'}) I'_{1v} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R' \times R'}) \rho'(s) \right)} = \quad (70)$$

for all $s \geq 0$.

Proof. First we notice that from the Campbell-Baker-Hausdorff formula, we have:

$$(e^{i\sigma_z t} \otimes \mathbf{1}_{R \times R}) I_{1v} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R \times R}) = \sum_{k=0}^{\infty} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R \times R}}^k I_{1v} \right) \frac{t^k}{k!}, \forall v \in \{x, y, z\}, \quad (71)$$

and an analogous equation for Σ' . Moreover, by applying Lemma 7.1 in Appendix A, with $W = I_{1v}$, $W' = I'_{1v}$, and $k = 1$, $v = z$, we have:

$$\text{Tr} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R \times R}} I_{1v} \rho(s) \right) = \text{Tr} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R' \times R'}} I'_{1v} \rho'(s) \right).$$

Now we can apply again Lemma 7.1 to the previous equality, to get:

$$\text{Tr} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R \times R}}^2 I_{1v} \rho(s) \right) = \text{Tr} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R' \times R'}}^2 I'_{1v} \rho'(s) \right).$$

By applying repeatedly this procedure we obtain:

$$\text{Tr} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R \times R}}^k I_{1v} \rho(s) \right) = \text{Tr} \left(\text{ad}_{i\sigma_z \otimes \mathbf{1}_{R' \times R'}}^k I'_{1v} \rho'(s) \right),$$

for all $k \geq 0$. Using this in (71), equation (70) follows. \square

The proof of the following lemma is given in Appendix A

Lemma 5.3 The following formula holds:

$$(e^{i\sigma_z t} \otimes \mathbf{1}_{R \times R}) I_{1x} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R \times R}) := P_{N_1}(t) \otimes \mathbf{1}_{R \times R}, \quad (72)$$

where the matrix $P_{N_1}(\cdot)$ is periodic with period 2π . Moreover

$$P_{N_1}(\pi) = -P_{N_1}(0) = -\sigma_x. \quad (73)$$

Using Lemmas 5.2 and 5.3, we can now conclude the proof that the spins are the same. Let $\bar{\rho}(s) \otimes \mathbf{1}_{R \times R}$ (resp. $\bar{\rho}'(s) \otimes \mathbf{1}_{R' \times R'}$) the orthogonal component of $\rho(s)$ (resp. $\rho'(s)$) along $\sigma_x \otimes \mathbf{1}_{R \times R}$ (resp. $\sigma_x \otimes \mathbf{1}_{R' \times R'}$). Using equation (72), equality (70) with $v = x$ can be written as :

$$\text{Tr} (P_{N_1}(t) \bar{\rho}(s)) R = \text{Tr} (P_{N'_1}(t) \bar{\rho}'(s)) R'. \quad (74)$$

Since we have assumed by contradiction $R > R'$, from (74) we have for every t :

$$\text{Tr} (P_{N_1}(t) \bar{\rho}(s)) < \text{Tr} (P_{N'_1}(t) \bar{\rho}'(s)). \quad (75)$$

Now we will derive a contradiction by evaluating the previous inequality at $t = 0$ and $t = \pi$ and using (73). In fact we have:

$$\text{Tr} (P_{N_1}(0) \bar{\rho}(s)) < \text{Tr} (P_{N'_1}(0) \bar{\rho}'(s)),$$

thus

$$\text{Tr} (P_{N_1}(\pi) \bar{\rho}(s)) = -\text{Tr} (P_{N_1}(0) \bar{\rho}(s)) > -\text{Tr} (P_{N'_1}(0) \bar{\rho}'(s)) = \text{Tr} (P_{N'_1}(\pi) \bar{\rho}'(s)).$$

The previous inequality contradicts equation (75). Thus we conclude that $l_1 = l'_1$, which implies that equation (58) holds.

Since the two equivalent models Σ and Σ' have the same spin, the positive constant α in (69) is equal to one. Therefore, for every pair $d, k \in \{1, \dots, n\}$, J_{dk} and J'_{dk} only differ possibly by the a sign factor. Using the same argument as in the main Theorem of [2] we can in fact conclude that there are only two possible case: The case where $J_{dk} = J'_{dk}$ for every pair d, k and the case where $J_{dk} = -J'_{dk}$ for every pair d, k . If we are in the first case, then from the observability (which follows from controllability) of the model, we must have $\rho_0 = \rho'_0$, thus equation (59) holds. This would be the case *a* of part 4. of Condition (*). On the other hand, if $J'_{kd} = -J_{kd}$ for every pair $1 \leq k < d \leq n$, we may conclude using Theorem 1. In fact we consider the homomorphism ϕ given by the Cartan involution associated to the odd-even decomposition as in the previous part of the proof. Conditions (9) hold, thus, since the models are equivalent and observable, we get that:

$$i\rho'_0 = \phi(i\rho_0),$$

thus equation (60) holds. This concludes the proof of the Theorem.

6 Proofs of Theorems 4-6

In the proofs of Theorems 4 and 5, we shall use the following two types of elementary $k \times k$ matrices:

$$C_k := \text{diag}(-1, 1, -1, \dots, (-1)^k), \quad T_k = \text{adiag}(1, 1, 1, \dots, 1). \quad (76)$$

The matrix C_k is diagonal with alternating elements while T_k is antidiagonal with all ones on the secondary diagonal and zeros everywhere else. Obvious properties of these matrices are the following

$$C_k^2 = T_k^2 = \mathbf{1}_{k \times k}, \quad T_k = T_k^T. \quad (77)$$

We are interested in the action of these matrices by similarity transformation on diagonal and tridiagonal $k \times k$ matrices. In particular, let us denote by D a generic, real, diagonal, $k \times k$ matrix and by F a generic, real, $k \times k$, tridiagonal matrix, which is also symmetric and it has zero diagonal. If M^a denotes the antitransposed of M , namely the matrix obtained by reflecting about the secondary diagonal, we can easily verify the following properties.

1.

$$C_k D C_k = D, \quad C_k F C_k = -F, \quad (78)$$

2.

$$T_k D T_k = D^a, \quad T_k F T_k = F^a. \quad (79)$$

Now we are ready to prove Theorems 4 and 5.

Proof of Theorem 4 The matrices $i\sigma_z$ and $i\sigma_x$ have (for every value of the spin) the following structure

$$i\sigma_z = i \begin{pmatrix} D & 0 \\ 0 & -D^a \end{pmatrix}, \quad (80)$$

$$i\sigma_x = i \begin{pmatrix} F & P \\ P^T & F^a \end{pmatrix}, \quad (81)$$

where F and D have the structure above specified with $k := \frac{N_j}{2}$ and P is a $k \times k$ real matrix of all zeros except in the $(k, 1)$ -th position. Now use

$$U := \begin{pmatrix} C_k & 0 \\ 0 & T_k \end{pmatrix}, \quad (82)$$

which is orthogonal and therefore unitary.

We calculate, using the first ones of (78) and (79)

$$i\tilde{\sigma}_z := Ui\sigma_zU^* = i \begin{pmatrix} D & 0 \\ 0 & -D \end{pmatrix}. \quad (83)$$

Moreover, using the second ones of (78) and (79), we have

$$i\tilde{\sigma}_x := Ui\sigma_xU^* = i \begin{pmatrix} -F & C_kPT_k \\ T_kPC_k & F \end{pmatrix}. \quad (84)$$

It is easily seen that $i\tilde{\sigma}_z$ and $i\tilde{\sigma}_x$ are symplectic, by observing that C_kPT_k is a real symmetric matrix (only the (k, k) -th element is different from zero). Therefore $sp(\frac{N_j}{2})$ contains a subalgebra conjugate to the one spanned by $i\sigma_x$ and $i\sigma_z$ and therefore $i\sigma_y$ and the Theorem is proved. \square

We now proceed to the proof of Theorem 5.

Proof of Theorem 5 In this case we set $k := \frac{N_j-1}{2}$. The matrix $i\sigma_z$ has the form

$$i\sigma_z := i \begin{pmatrix} -D & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D^a \end{pmatrix}, \quad (85)$$

with D of dimension $k \times k$. Moreover $i\sigma_x$ has the form

$$i\sigma_x := i \begin{pmatrix} F & v & 0 \\ v^T & 0 & w^t \\ 0 & w & F^a \end{pmatrix}, \quad (86)$$

where F is as above and v (w) is a vector of dimension k with only the last (the first) component different from zero, and the components different from zero are equal for v and w . We use the unitary matrix

$$U := \begin{pmatrix} \frac{i}{\sqrt{2}}C_k & 0 & (-1)^k \frac{i}{\sqrt{2}}T_k \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}}T_k & 0 & \frac{1}{\sqrt{2}}C_k \end{pmatrix}, \quad (87)$$

which is easily seen to be unitary by (76) (77). We calculate.

$$i\tilde{\sigma}_z := Ui\sigma_zU^* = i \begin{pmatrix} \frac{1}{2}(T_kD^aT_k - C_kDC_k) & 0 & \frac{i}{2}((-1)^kT_kD^aC_k - C_kDT_k) \\ 0 & 0 & 0 \\ \frac{i}{2}(T_kDC_k - (-1)^kC_kD^2T_k) & 0 & \frac{1}{2}(C_kD^aC_k - T_kDT_k) \end{pmatrix}. \quad (88)$$

Using the first ones of (78) and (79), we find that the diagonal blocks are zero. Moreover, the remaining elements of the matrix are real so that $i\tilde{\sigma}_z$ is real. Analogously, we calculate

$$i\tilde{\sigma}_x := Ui\sigma_xU^* = \quad (89)$$

$$i \begin{pmatrix} \frac{1}{2}(C_k F C_k + (-1)^{2k} T_k F^a T_k) & \frac{i}{\sqrt{2}}(C_k v + (-1)^k T_k w) & \frac{i}{2}(C_k F T_k + (-1)^k T_k F^a C_k) \\ * & 0 & \frac{1}{\sqrt{2}}(v^T T_k + w^T C_k) \\ * & * & \frac{1}{2}(T_k F T_k + C_k F^a C_k) \end{pmatrix},$$

where we have denoted by a star $*$ the components that can be obtained from the requirement that the matrix is skew Hermitian. Now the $(1, 1)$ and $(3, 3)$ blocks are zero from the second ones of properties (78) and (79), while the $(2, 3)$ block is zero because of the structure of the vectors v and w . All the other blocks are purely real matrices so that $i\tilde{\sigma}_x$ is also in $so(n)$ and this completes the proof. \square

We now give the proof of the negative result in Theorem 6.

Proof of Theorem 6 Assume that there exists a matrix $X \in SU(N_j)$ such that

$$Xi\sigma_x X^* := \tilde{R}_x, \quad (90)$$

$$Xi\sigma_y X^* := \tilde{R}_y, \quad (91)$$

$$Xi\sigma_z X^* := \tilde{R}_z, \quad (92)$$

with \tilde{R}_x , \tilde{R}_y and \tilde{R}_z in $so(N_j)$. Then we can use the **AI** Cartan decomposition of $SU(N_j)$ [9] to write X as

$$X = K_1 A K_2, \quad (93)$$

with K_1 and K_2 in $SO(N_j)$ and A diagonal i.e.

$$A := \text{diag}(e^{i\phi_1}, \dots, e^{\frac{i\phi_{N_j}}{2}}). \quad (94)$$

Therefore we can write

$$K_1 A K_2 i\sigma_{x,y,z} K_2^T \bar{A} K_1^T = \tilde{R}_{x,y,z}, \quad (95)$$

or, defining $R_{x,y,z} := K_1^T \tilde{R}_{x,y,z} K_1$ which is also real skew-symmetric, we can write

$$K_2 i\sigma_{x,y,z} K_2^T = \bar{A} R_{x,y,z} A. \quad (96)$$

The real matrices $R_{x,y,z}$ must satisfy the same basic commutation relations (35) of $i\sigma_x$, $i\sigma_y$ and $i\sigma_z$ and have the same eigenvalues of $i\sigma_x$, $i\sigma_y$ and $i\sigma_z$, namely for a (half integer) spin j , $\pm j i$, $\pm(j+1)i, \dots, \pm \frac{1}{2}i$. We now study the structure of $R_{x,y,z}$ in (96) and get a contradiction with these facts.

First notice that, since A is diagonal as in (94), the action of A on the right hand side of (96) namely, $R \rightarrow \bar{A} R A$ changes the (real) element r_{jk} of R into $r_{jk} e^{-i(\phi_j - \phi_k)}$. Since the entries on the left hand side of (96) are either all purely imaginary or all purely real, if $\phi_j - \phi_k$ is not a multiple of $\frac{\pi}{2}$ then we must have $r_{jk} = 0$. Consider the indices $1, \dots, N_j$ and let \mathcal{O} be the set of indices k such that $\phi_1 - \phi_k$ is an odd multiple of $\frac{\pi}{2}$ and \mathcal{E} the set of indices k such that $\phi_1 - \phi_k$ is an even multiple of $\frac{\pi}{2}$, and \mathcal{N} the set of indices k such that $\phi_1 - \phi_k$ is not an integer multiple of $\frac{\pi}{2}$.

From (96) it follows that since $i\sigma_y$ is real the terms r_{jk} of R_y where j and k belong to different sets must be zero because in that case $e^{i(\phi_j - \phi_k)}$ in (94) has a nonzero imaginary part in this case. Therefore only the elements r_{jk} where j and k belongs both to \mathcal{O} , or both to \mathcal{E} , or both to \mathcal{N} , are possibly different from zero. Therefore after possibly a reordering of rows and columns, which corresponds to a similarity transformation by a permutation matrix, R_y must be of block diagonal form and without loss of generality and for simplicity we shall assume only two blocks (rather than three). Therefore we write

$$R_y := \begin{pmatrix} Y_{11} & 0 \\ 0 & Y_{22} \end{pmatrix}, \quad (97)$$

where Y_{11} has dimensions $n_o \times n_o$ with n_o the cardinality of \mathcal{O} and Y_{22} has dimension $(n - n_o) \times (n - n_o)$. Both Y_{11} and Y_{22} are skew-symmetric matrices. An analogous argument shows that, after possibly the same re-ordering of column and row indices, R_z can be written as

$$R_z : \begin{pmatrix} 0 & Z_{12} \\ -Z_{12}^T & 0 \end{pmatrix}, \quad (98)$$

where Z_{12} is a general matrix of dimensions $n_o \times (n - n_o)$.

Now consider the possible values for n_o . n_o odd is to be excluded because this would cause $\det Y_{11} = 0$ in (97) and this contradicts the fact that R_y has no zero eigenvalues. Moreover $n_o \neq (n - n_o)$ (i.e. $n_o \neq \frac{N_j}{2}$) would cause R_z to have determinant equal to zero. This can be easily verified by calculating

$$\det(R_z^2) = (\det R_z)^2 = \det \begin{pmatrix} -Z_{12}Z_{12}^T & 0 \\ 0 & -Z_{12}^TZ_{12} \end{pmatrix}, \quad (99)$$

since, in this case, at least one of the matrices on the diagonal blocks does not have full rank. These considerations already exclude the cases where $\frac{N_j}{2}$ is an odd number as for spins $\frac{1}{2}$, $\frac{5}{2}$, $\frac{9}{2}$ etc. and we can assume R_y and R_z of the form (97) and (98) with $n_o = \frac{N_j}{2}$. To obtain a contradiction in this case too we first notice that, since Y_{11} and Y_{22} have even dimension and are skew-symmetric, we can apply a similarity transformation $T := \begin{pmatrix} T_1 & 0 \\ 0 & T_2 \end{pmatrix}$, with T_1 and T_2 orthogonal so that TR_yT^T is block diagonal

$$TR_yT^T = (D_1, D_2, \dots, D_{\frac{N_j}{2}}), \quad (100)$$

where the 2×2 block D_k has the form

$$D_k := \begin{pmatrix} 0 & l_k \\ -l_k & 0 \end{pmatrix}, \quad (101)$$

where each l_k corresponds to a couple of complex conjugate eigenvalues of R_y so that $l_k = \frac{p}{2}$ with p odd corresponds to the pair $\pm \frac{p}{2}i$. Moreover we choose T so that the first $\frac{N_j}{4}$ blocks are ordered according to the increasing value of l_k and the same thing for the last $\frac{N_j}{4}$ blocks. We shall therefore assume this structure of R_y in the remainder of the proof. We notice also that the transformation TR_zT^T does not change the structure of R_z as Z_{12} in (98) was chosen to be a general $\frac{N_j}{2} \times \frac{N_j}{2}$ real matrix. Express Z_{12} in terms of 2×2 blocks L_{fk} , $f, k = 1, \dots, \frac{N_j}{4}$, $k = \frac{N_j}{4} + 1, \dots, \frac{N_j}{2}$, which is possible since $\frac{N_j}{2}$ is an even number. Now, we impose the fact that R_y and R_z have to satisfy the same commutation relations as $i\sigma_y$ and $i\sigma_z$. In particular, we must have

$$[[R_y, R_z], R_y] = R_z. \quad (102)$$

This equation gives for the L_{fk} block the following one

$$2D_f L_{fk} D_k - L_{fk} D_k^2 - D_f^2 L_{fk} = L_{fk}. \quad (103)$$

If we write the generic L_{fk} as

$$L_{fk} := \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}, \quad (104)$$

and recall the structure of D_f and D_k ,

$$D_f := \begin{pmatrix} 0 & l_f \\ -l_f & 0 \end{pmatrix}, \quad D_k := \begin{pmatrix} 0 & l_k \\ -l_k & 0 \end{pmatrix}, \quad (105)$$

we obtain the following equations for a_2 and a_3 (and analogous equations for a_1 and a_4)

$$2l_k l_f a_3 = (1 - l_f^2 - l_k^2) a_2, \quad (106)$$

$$2l_k l_f a_2 = (1 - l_f^2 - l_k^2) a_3. \quad (107)$$

Combining these, we obtain

$$4l_k^2 l_f^2 a_3 = (1 - l_k^2 - l_f^2)^2 a_3, \quad (108)$$

which shows, taking the square root of both sides, that the only possibilities to have a_3 and therefore a_2 different from zero are the cases $l_f + l_k = \pm 1$. In these cases we can easily see that

$$a_3 = -a_2. \quad (109)$$

Similarly, one finds that we have a_4 and a_1 in (104) different from zero if and only if $l_f + l_k = \pm 1$ and, in these cases we have

$$a_1 = a_4. \quad (110)$$

In conclusion, all the blocks L_{fk} are zero except the ones corresponding to indices f and k with neighboring values of l_f and l_k which have the structure

$$L_{fk} := \begin{pmatrix} x & y \\ -y & x \end{pmatrix}. \quad (111)$$

Therefore R_z has the form in (98) where the f -th block row of Z_{12} has at most two blocks different from zero and with the structure in (111). We denote these blocks by P_f and S_f , where P (S) stands for 'predecessor' ('successor') and correspond to the index k such that $l_k = l_f - 1$ and $l_k = l_f + 1$, respectively. Now, we argue that a matrix R_z with this structure must necessarily have all the (purely imaginary) eigenvalues with multiplicity at least two and this gives the desired contradiction because R_z should have the same spectrum of $i\sigma_{x,y,z}$ which consists of all simple eigenvalues. In order to see this fact, re-consider the block structure of R_y in (100). If the blocks corresponding to eigenvalues $\pm \frac{1}{2}i$ and $\pm \frac{3}{2}i$ belong to the same half, then the corresponding matrix R_z will have a two dimensional block row (or column) equal to zero, and therefore 0 will be an eigenvalue with multiplicity at least 2. Therefore we can assume that these two blocks belong to two different halves and by the ordering we have imposed they must be the first ones of each half. Assume that the block corresponding to $\pm \frac{1}{2}i$ is in the first half. If this is not the case, consider the transposed of R_z and repeat the arguments that follow. It is possible to choose a block diagonal similarity transformation

$$U := \text{diag}(G_1, G_2, \dots, G_{\frac{N_i}{4}}, F_1, F_2, \dots, F_{\frac{N_i}{4}}), \quad (112)$$

with all the G_f 's and F_f 's 2×2 orthogonal matrices so that $UR_z U^T$ has the same structure as before but all the matrices P_j and S_j are *scalar* matrices. We construct the matrix U proceeding by block rows. The first block row contains only S_1 as $\frac{1}{2}$ has no predecessors. All the zero blocks remain zero and S_1 is transformed as

$$G_1 S_1 F_1^T. \quad (113)$$

We choose $F_1 = \mathbf{1}_{2 \times 2}$ and G_1 , which has the general form

$$G_1 := \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}, \quad (114)$$

so that $\sin(\theta)x + \cos(\theta)y = 0$ if $S_1 := \begin{pmatrix} x & y \\ -y & x \end{pmatrix}$. This will give a scalar matrix. At the generic f -th block row, we have, at the most two nonzero blocks P_{fk} and S_{fb} where we now use an extra index k and b to indicate the block column to which they belong. They transform as

$$P_{fk} \rightarrow G_f P_{fk} F_k^T, \quad (115)$$

and

$$S_{fb} \rightarrow G_f S_{fb} F_b^T, \quad (116)$$

respectively, while all the other blocks remain zero. If F_k has not been chosen before we set $F_k = \mathbf{1}_{2 \times 2}$. In any case, we choose G_f as before to make $G_f P_{fk} F_k^T$ a scalar matrix. We then choose F_b to make $G_f S_{fb} F_b^T$ a scalar matrix. G_f and F_b had not been chosen at previous steps. This is obvious for G_f and follows by an induction argument for F_b since all the F matrices chosen before the f -th step correspond to predecessors and successors with (column) indices strictly less than b (recall that in the two halves of the matrix R_y the blocks are arranged in increasing order of (absolute value of) eigenvalue). In conclusion, modulo the similarity transformation defined by U in (112), we can assume that R_z has the form

$$R_z = K \otimes I_{2 \times 2}, \quad (117)$$

where K is a skew-symmetric $\frac{N_j}{2} \times \frac{N_j}{2}$ matrix. By known results on the eigenvalues of the Kronecker products of two matrices, it follows that the eigenvalues of R_z are the same as those of K each with multiplicity at least two. This gives the desired contradiction and concludes the proof of the Theorem. \square

7 Conclusions

This paper has presented a collection of mathematical results concerning the input-output equivalence of quantum systems. Models that are equivalent cannot be distinguished by an external observer and therefore the determination of parameters in a quantum Hamiltonian can only be obtained up to equivalent models. Motivated by recent results on the isospectrality of quantum Hamiltonians [14] in molecular magnets, we have completely characterized the classes of spin networks which are equivalent. In several cases, the characterization of equivalent models can be obtained through a Lie algebra homomorphism which is suggested by a Cartan structure of the underlying dynamics.

We believe many of the results and the concepts presented in this paper for quantum systems could be generalized to classes of systems relevant in other applications with both dynamics and output linear in the state. This will be the subject of further research.

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Appendix A: Additional results and proofs

The proof of the following Lemma can be obtained with a formal modification of the proof of Lemma 4.4 in [2] and it is therefore omitted.

Lemma 7.1 Let Σ and Σ' be two equivalent models. If W and W' are two given Hermitian matrices such that

$$\text{Tr}(W\rho(t)) = \text{Tr}(W'\rho'(t)), \quad (118)$$

for every pair of corresponding trajectories $\rho(t)$ and $\rho'(t)$, then it also holds

$$\text{Tr}([W, I_{kv}]\rho(t)) = \text{Tr}([W', I'_{(k)v}]\rho'(t)), \quad \forall k \in \{1, \dots, n\}, \forall v \in \{x, y, z\}, \quad (119)$$

up to a permutation of the indices ⁷.

⁷This permutation is the same and fixed for all the results where it is mentioned

Proof of Lemma 5.1

We first state a Lemma whose proof can be obtained from the proof of Lemma 5.1 in [2] and then proceed to the proof of Lemma 5.1

Lemma 7.2 Assume that for all $t \geq 0$, all the possible trajectories $\rho(t)$ of Σ and corresponding $\rho'(t)$ of Σ' , for fixed values $1 \leq k_1, \dots, k_r \leq n$, and fixed $v_j \in \{x, y, z\}$, we have:

$$\text{Tr}(I_{k_1 v_1, \dots, k_r v_r} \rho(t)) = \text{Tr}(I'_{k_1 v_1, \dots, k_r v_r} \rho'(t)). \quad (120)$$

Then:

1. equation (120) holds for any possible choice of the values of $v_j \in \{x, y, z\}$;

2.

$$\begin{aligned} & \text{Tr} \left(\left[\left[iI_{\bar{d}v_{\bar{d}}}, [iI_{\bar{k}v_{\bar{k}}}, A] \right], I_{k_1 v_1, \dots, k_r v_r} \right] \rho(t) \right) = \\ & \text{Tr} \left(\left[\left[iI'_{\bar{d}v_{\bar{d}}}, [iI'_{\bar{k}v_{\bar{k}}}, A'] \right], I'_{k_1 v_1, \dots, k_r v_r} \right] \rho'(t) \right), \end{aligned} \quad (121)$$

for all the indices $1 \leq \bar{d} \neq \bar{k} \leq n$ and every $\{v_{\bar{d}} \neq v_{\bar{k}}\} \in \{x, y, z\}$.

We now proceed to the proof of Lemma 5.1. First notice that from Lemma 7.2, it is enough to prove (65) and (66) for a particular choice of $\{v_j\}$ and \bar{v} . Moreover, we have, for $\bar{d} > \bar{k}$,

$$[iI_{\bar{d}z}, [iI_{\bar{k}x}, A]] = -J_{\bar{k}\bar{d}} iI_{\bar{k}z, \bar{d}x}. \quad (122)$$

1. By applying Lemma 7.2 (equation (121)) to (64) and using (122) we get:

$$\beta \text{Tr} \left([-J_{\bar{k}\bar{d}} iI_{\bar{k}z, \bar{d}x}, I_{k_1 v_1, \dots, k_r v_r}] \rho(t) \right) = \beta' \text{Tr} \left(\left[-J'_{\bar{k}\bar{d}} iI'_{\bar{k}z, \bar{d}x}, I'_{k_1 v_1, \dots, k_r v_r} \right] \rho'(t) \right). \quad (123)$$

We may assume, without loss of generality, that $\bar{k} = k_j$ and $v_j = x$. In this case we have:

$$-J_{\bar{k}\bar{d}} [iI_{\bar{k}z, \bar{d}x}, I_{k_1 v_1, \dots, k_r v_r}] = J_{\bar{k}\bar{d}} iI_{k_1 v_1, \dots, k_j y, \dots, k_r v_r, \bar{d}x}.$$

Combining the previous equality with (123), equation (65) follows easily.

2. Using the same procedure, we obtain again equation (123), but now both indices \bar{k} and \bar{d} are in $\{k_1, \dots, k_r\}$. Assume, for example that $k_1 = \bar{k}$ and $k_2 = \bar{d}$, and take $v_{k_1} = v_{k_2} = x$.

Now we have:

$$[I_{k_1 z, k_2 x}, I_{k_1 x, k_2 x, \dots, k_r v_r}] = I_{k_1 y, k_2 x^2, k_3 v_3, \dots, k_r v_r}, \quad (124)$$

where, with this notation, we mean that in the k_2^{th} position we have the matrix σ_x^2 . Thus, combining equations (123) and (124), we get:

$$\beta J_{k_1 k_2} \text{Tr}(I_{k_1 y, k_2 x^2, k_3 v_3, \dots, k_r v_r} \rho(t)) = \beta' J'_{k_1 k_2} \text{Tr}(I'_{k_1 y, k_2 x^2, k_3 v_3, \dots, k_r v_r} \rho'(t)). \quad (125)$$

Using the same procedure, we conclude:

$$\beta J_{k_1 k_2} \text{Tr}(I_{k_1 y, k_2 y^2, k_3 v_3, \dots, k_r v_r} \rho(t)) = \beta' J'_{k_1 k_2} \text{Tr}(I'_{k_1 y, k_2 y^2, k_3 v_3, \dots, k_r v_r} \rho'(t)), \quad (126)$$

and

$$\beta J_{k_1 k_2} \text{Tr}(I_{k_1 y, k_2 z^2, k_3 v_3, \dots, k_r v_r} \rho(t)) = \beta' J'_{k_1 k_2} \text{Tr}(I'_{k_1 y, k_2 z^2, k_3 v_3, \dots, k_r v_r} \rho'(t)). \quad (127)$$

Adding together equations (125), (126), and (127) and using (52), we get:

$$\beta(l_{k_2}(l_{k_2} + 1))J_{k_1 k_2} \text{Tr}(I_{k_1 y, k_3 v_3, \dots, k_r v_r} \rho(t)) = \beta'(l'_{k_2}(l'_{k_2} + 1))J'_{k_1 k_2} \text{Tr}(I'_{k_1 y, k_3 v_3, \dots, k_r v_r} \rho'(t)),$$

as desired.

Proof of Lemma 5.3

Proof.

We recall the formulas (72) and (73) to be proved, i.e.:

$$(e^{i\sigma_z t} \otimes \mathbf{1}_{R \times R}) I_{1x} (e^{-i\sigma_z t} \otimes \mathbf{1}_{R \times R}) := P_{N_1}(t) \otimes \mathbf{1}_{R \times R}, \quad (128)$$

where the matrix $P(\cdot)$ is periodic with period 2π , and

$$P_{N_1}(\pi) = -P_{N_1}(0) = \sigma_x. \quad (129)$$

The proof can be done directly by computing the matrix above. This is simplified by the fact that the matrix σ_z is always a diagonal matrix. We will give an outline of the argument when l_1 is half integer spin. The idea is to use the representations for the matrices σ_z and σ_x given by equations (80) and (81). The case of integer spin can be derived similarly starting with the representations given by equations (85) and (86).

Using equations (80) and (81), we obtain

$$e^{i\sigma_z t} i\sigma_x e^{-i\sigma_z t} = \begin{pmatrix} e^{iDt} F e^{-iDt} & e^{iDt} P e^{iD^a t} \\ e^{iD^a t} P^T e^{-iDt} & e^{-iD^a t} F^a e^{iD^a t} \end{pmatrix}. \quad (130)$$

The properties of the matrices D , P and F are described in Section 6. Moreover $D = \text{diag}(j, j-1, \dots, \frac{1}{2})$ for a half integer spin j . By using these properties, it follows that all the time depending terms in equation (130) are of the form e^{it} . Thus matrix (130) is periodic of period 2π . The fact that the dependence is of the type e^{it} , in turn, implies that equations (128) and (129) hold.

□